

# Towards finite density QCD with Taylor expansions

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Convergence properties of Taylor expansions of observables, which are also used in lattice QCD calculations at non-zero chemical potential, are analyzed in an effective  $N_f = 2 + 1$  flavor Polyakov-quark-meson model. A recently developed algorithmic technique allows the calculation of higher-order Taylor expansion coefficients in functional approaches. This novel technique is for the first time applied to an effective  $N_f = 2 + 1$  flavor Polyakov-quark-meson model and the findings are compared with the full model solution at finite densities. The results are used to discuss prospects for locating the QCD phase boundary and a possible critical endpoint in the phase diagram.

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## I. INTRODUCTION

Exploring chiral and deconfining properties of strongly-interacting matter at high temperature is one of the most interesting issues in modern physics (for reviews, see e.g. [1–3]). In particular, the possible existence of a critical endpoint (CEP) in the QCD phase diagram at non-zero net baryon number density and its consequences for the phase structure of QCD at lower temperatures are much under debate, e.g. [4]. High energy heavy-ion collision experiments at RHIC and SPS started to look for experimental evidence of the CEP and experiments at new heavy-ion facilities (FAIR and NICA), have been designed to probe the relevant high density region in the QCD phase diagram.

Gaining insight into properties of QCD at non-zero, even small values of the quark chemical potential ( $\mu$ ) is thus of great interest. However, in theoretical calculations the relevant region in the QCD phase diagram is not easy to access directly in QCD. Model calculations or non-perturbative lattice QCD calculations, based on approximation schemes, are currently used.

At vanishing chemical potential the lattice QCD calculations get refined systematically and become possible with almost realistic quark mass values. They indicate a temperature-driven crossover transition from hadrons to the quark-gluon-plasma phase, for a recent review see [5].

However, even in this case the quantitative determination of the transition temperature is still a difficult task. A careful analysis of cut-off effects is needed to extract this quantity in the continuum limit [6, 7].

At non-zero values of the chemical potential the notorious fermion sign problem prohibits straightforward lattice QCD simulations. In order to enter at least the small chemical potential region of the QCD phase diagram several extrapolation methods such as the reweighting technique, analytic continuation to imaginary chemical potential or Taylor series expansions have been proposed. All these extrapolation methods have their own, intrinsic problems and their reliability is still under investigation, see e.g. [8–10] for reviews. Under these circumstances, it may be useful to apply approximation schemes, used currently in lattice QCD calculations, also in model calculations. Through a comparison with analytic results obtainable in QCD-like models, insight may be gained for the application of approximation schemes in lattice QCD calculations.

In this work we focus on the Taylor expansion technique where a thermodynamic quantity such as the pressure is expanded in powers of the chemical potential  $\mu$  around vanishing chemical potential, i.e., around the point at which Monte Carlo simulations are not hindered by the sign problem. This method was developed for studies of QCD thermodynamics with the aim to gain information also on the location of a possible critical point in the QCD phase diagram [11, 12]. In general, the relevant Taylor coefficients can be calculated with standard simulation techniques used also at  $\mu = 0$  [13–15]. With this approach the calculation of several thermodynamic quantities has been extended to non-zero values of the chemical potential; results have been compared with hadron resonance gas model calculations at low temperature [16] and quark-gluon gas thermodynamics at high temperature. Attempts have also been made to determine the phase boundary and to infer a possible critical endpoint in the phase diagram from convergence properties of the Taylor series for thermodynamic quantities, e.g., the pressure or quark number suscepti-

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bility [9, 11, 12, 17].

So far, basic features of the Taylor series such as its convergence properties have received only little attention because a proper investigation of these aspects requires the knowledge of higher-order Taylor coefficients. In most QCD studies these coefficients are difficult to obtain and a systematic analysis of convergence properties is not yet possible. At present any attempts to identify some precursor effects of a possible critical endpoint thus have to rely on information extracted from a few low order expansion coefficients.

Recently, a new algorithmic differentiation technique has been developed that allows for the calculation of higher-order Taylor coefficients in functional approaches [18]. This enables one to investigate general convergence properties of the Taylor expansion method at least in model calculations. Their consequences and prospects for the determination of the phase boundary and a possible critical endpoint are discussed here in the framework of the effective  $N_f = 2 + 1$  flavor Polyakov-quark-meson (PQM) model. The model is studied in mean-field approximation and the findings from the Taylor expansion are compared with the corresponding model mean-field solution at finite density [19].

The outline of this work is as follows: In Sec. II the Taylor expansion method and its application to the analysis of different approximants for radii of convergence are introduced. We also discuss the improvement of Taylor series expansions by a Padé resummation. Basic strategies for the determination of the phase boundary and the location of a critical endpoint in the phase diagram from Taylor expansion coefficients are discussed in Sec. III. Sec. IV is devoted to the presentation of the model analysis where higher-order Taylor coefficients are used to locate the phase boundary and the critical endpoint at finite chemical potential. We conclude in Sec. V with a brief summary and discussion of our findings.

## II. EXTRAPOLATION TO FINITE $\mu$

The Taylor expansion method has been used as an approximation scheme to gain information on QCD thermodynamics at high temperature and for small, non-vanishing values of the chemical potential. Here, we start with a description of some generic model-independent properties of the Taylor expansion of, e.g., the QCD partition function (see also [20]).

### A. Taylor expansion

At fixed temperature the logarithm of the QCD partition function, *i.e.* the pressure  $p = (T/V) \ln \mathcal{Z}$ , may be expanded in a Taylor series in powers of  $\mu/T$

around  $\mu = 0$ :

$$\frac{p(\mu/T)}{T^4} = \sum_{n=0}^{\infty} c_n(T) \left(\frac{\mu}{T}\right)^n. \quad (1)$$

The Taylor expansion coefficients are determined by derivatives with respect to the chemical potential evaluated at vanishing  $\mu$ ,

$$c_n(T) = \frac{1}{n!} \left. \frac{\partial^n (p(T, \mu)/T^4)}{\partial (\mu/T)^n} \right|_{\mu=0}. \quad (2)$$

Due to the CP-symmetry of QCD, the partition function is symmetric in  $\mu$ , *i.e.*  $\mathcal{Z}(\mu) = \mathcal{Z}(-\mu)$  which reflects the invariance of  $\mathcal{Z}$  under exchange of particles and antiparticles. As a consequence, all odd expansion coefficients vanish and the series is even in  $\mu/T$ . In QCD, various quark chemical potentials have to be taken into account in this expansion. However, in order to simplify our discussion in the following, we focus on one uniform quark chemical potential  $\mu \equiv \mu_q = \mu_B/3$  which will not restrict our conclusions.

Besides the pressure, any thermodynamic observables like, e.g., the energy density ( $\epsilon$ ), the trace anomaly ( $\epsilon - 3p$ ) or the quark number susceptibility  $\chi_q$  can be expanded in a similar series with appropriately modified Taylor expansion coefficients [17, 21]. Of course, all these modified Taylor expansion coefficients are related to the initial expansion coefficients of the pressure. An instructive example is the Taylor expansion of the quark number susceptibility,  $\chi_q$ , which is defined as the second derivative of the pressure w.r.t. to  $\mu$

$$\chi_q(T, \mu) = \frac{\partial^2 p(T, \mu)}{\partial \mu^2}. \quad (3)$$

This yields the following relation to the corresponding Taylor expansion coefficients  $c_n(T)$  of the pressure

$$\frac{\chi_q(\mu/T)}{T^2} = \sum_{n=2}^{\infty} \underbrace{n(n-1)c_n(T)}_{=c_{n-2}^x(T)} \left(\frac{\mu}{T}\right)^{n-2}. \quad (4)$$

The expansion of other thermodynamic quantities like, for instance, the trace anomaly requires additional derivatives of the Taylor coefficients w.r.t. the temperature.

In the following we compare the Taylor expansion of the pressure and the quark number susceptibility at non-zero chemical potential. If a critical endpoint exists in the QCD phase diagram then it is expected that the quark number susceptibility diverges at that point while the pressure stays finite and is still continuous. Although the Taylor series for both quantities have identical radii of convergence they thus will behave differently on the phase boundary. A comparison of both series as the truncation order is increased might therefore be helpful to gain new insights in locating a possible CEP in the QCD phase diagram.

## B. Radius of convergence

Whether or not the radius of convergence of the Taylor expansion of the thermodynamic potential around  $\mu = 0$  is related to a phase transition in the physical system crucially depends on the location of the singularity in the complex  $\mu$ -plane that causes the breakdown of the series expansion. Only if this singularity lies on the real axis the radius of convergence corresponds to the location of a critical point. Information on the location of the singularity in the complex  $\mu$ -plane can be deduced from properties of the Taylor expansion coefficients themselves. In any case, the singularity closest to  $\mu = 0$  will determine the radius of convergence of the Taylor series. This can be obtained from the behavior of the Taylor expansion coefficients of the pressure,

$$r = \lim_{n \rightarrow \infty} r_{2n} = \lim_{n \rightarrow \infty} \left| \frac{c_{2n}}{c_{2n+2}} \right|^{1/2}. \quad (5)$$

Other definitions of the radius of convergence are known and their application in the context of QCD have been discussed in the literature, see e.g. [12].

Of course, in almost all applications only a finite number of expansion coefficients are known and the limit  $n \rightarrow \infty$  cannot be performed. In some cases it might be possible to extrapolate the  $r_{2n}$  to infinity, making use of their expected asymptotic behavior. Otherwise, one will have to assume that the radius of convergence  $r$  has been reached when subsequent estimators,  $r_{2n}$ , do not change within errors anymore.

At a given order  $n$  the Taylor expansions of different observables will give different estimators for the radius of convergence, which are all related. For example, the estimator for the radius of convergence obtained from the quark number susceptibility,  $r_{2n}^X$ , is related to the one obtained from the pressure series via

$$r_{2n}^X = \left| \frac{c_{2n}^X}{c_{2n+2}^X} \right|^{1/2} = \left( \frac{(2n+2)(2n+1)}{(2n+3)(2n+4)} \right)^{1/2} r_{2n+2}. \quad (6)$$

In the limit  $n \rightarrow \infty$  both estimators for the radius of convergence will converge to the same unique limit  $r$  since the prefactor in front of  $r_{2n+2}$  tends to one. However, at finite order  $n$  the estimates for  $r_{2n}$  and  $r_{2n}^X$  will differ and as a consequence both may approach the limit  $r$  at a different rate. For large  $n$  we find from Eq. (6)

$$r_{2n}^X = r_{2n+2} \left( 1 - \frac{1}{n} + \mathcal{O}(n^{-2}) \right). \quad (7)$$

When deviations from the asymptotic value  $r$  are of  $\mathcal{O}(1/n)$ , i.e.,  $r_{2n+2} \simeq r(1 + A/n)$  with a positive, constant  $A$ , both estimators for the radius of convergence will converge with the same truncation errors of  $\mathcal{O}(1/n)$  (cf. App. A). Deviations from the asymptotic value  $r$  will, however, be numerically smaller in the susceptibility series than in the pressure series by a factor  $(A-1)/A$ . In other words, the estimator for the radius of convergence

obtained from the susceptibility series at given order  $n$  might be more suitable for estimating the true radius of convergence than the one obtained from other observables, e.g., from the pressure series.

## C. Resummations: Padé approximation

The convergence of a Taylor series can be improved further by a resummation of the expansion coefficients which is based on a Padé approximation (for details see [22]). For clarity and completeness, we collect the needed facts here. The Padé resummation employs the same derivative information as the initial Taylor expansion coefficients but often shows an extended convergence range, in particular in the presence of singularities. Furthermore, a more stable result can be achieved with fewer coefficients.

The Padé approximant can be obtained by rewriting a Taylor series of an analytic function  $t(x)$  around  $x_0 = 0$  to order  $N$

$$t(x) = \sum_{i=0}^N t_{(i)} x^i \quad (8)$$

as a ratio of two power series  $p(x)$  and  $q(x)$  of order  $L$  and  $M$ , respectively

$$[L/M] \equiv R_{L,M}(x) = \frac{p(x)}{q(x)} = \frac{p_0 + p_1 x + \dots + p_L x^L}{1 + q_1 x + \dots + q_M x^M}. \quad (9)$$

One advantage of this reformulation is that poles and singularities are better characterized by a rational function than by a polynomial Taylor series. The expansion coefficients for  $p$  and  $q$  can be obtained up to order  $N = L + M$  by equating the derivatives of both series up to order  $N$  at  $x = 0$ , i.e.,

$$\left. \frac{\partial^i R_{L,M}(x)}{\partial x^i} \right|_{x=0} = \left. \frac{\partial^i t(x)}{\partial x^i} \right|_{x=0} \quad \text{for } i \leq N. \quad (10)$$

An alternative and more elegant form relates the Padé approximant to determinants of two  $(M+1) \times (M+1)$  matrices as follows

$$[L/M] = \frac{\begin{vmatrix} t_{(L-M+1)} & t_{(L-M+2)} & \dots & t_{(L+1)} \\ t_{(L-M+2)} & t_{(L-M+3)} & \dots & t_{(L+2)} \\ \vdots & \vdots & \ddots & \vdots \\ t_{(L)} & t_{(L+1)} & \dots & t_{(L+M)} \\ \sum_{i=0}^{L-M} t_{(i)} x^{M+i} & \sum_{i=0}^{L-M+1} t_{(i)} x^{M+i-1} & \dots & \sum_{i=0}^L t_{(i)} x^i \end{vmatrix}}{\begin{vmatrix} t_{(L-M+1)} & t_{(L-M+2)} & \dots & t_{(L+1)} \\ t_{(L-M+2)} & t_{(L-M+3)} & \dots & t_{(L+2)} \\ \vdots & \vdots & \ddots & \vdots \\ t_{(L)} & t_{(L+1)} & \dots & t_{(L+M)} \\ x^M & x^{M-1} & \dots & 1 \end{vmatrix}}. \quad (11)$$

Note that for  $M = 0$  and  $L = N$  the Padé approximant is identical to the initial Taylor approximation, i.e.,

$[N/0] \equiv t(x)$ . Of course, apart from choosing the highest derivative order  $N$  in the Padé approximation one can also vary  $L$  or  $M$  independently.

The determination of the radius of convergence or the phase boundary with the Padé approximation is more involved. For the case  $[N/2]$  one immediately sees, Eq. (11), that the Padé approximant has a pole at  $x = \pm\sqrt{c_N/c_{N+2}}$  since the odd Taylor coefficients vanish. This pole coincides with the estimator for the radius of convergence,  $r_N$ , of the Taylor series up to order  $x^{N+2}$ , Eq. (5). For a general Padé approximant  $[L/M]$  the pole structure is more elaborated. However, in this case the first pole at positive and real chemical potential might provide a useful estimate for the phase boundary.

### III. LOCATING A CRITICAL ENDPOINT

It has been argued that the estimators for the radius of convergence can be used to determine the location of a possible CEP in the QCD phase diagram [11, 12, 23]. In general, a breakdown of a Taylor expansion is caused by a singularity in the complex  $\mu$ -plane. Only if this singularity, which is closest to the origin at  $\mu = 0$ , lies on the real  $\mu$ -axis, it is also related to a physical phase transition since it is a singularity in a thermodynamic quantity corresponding to a zero in the partition function [24]. If a CEP exists in the QCD phase diagram, it belongs to the universality class of the three dimensional Ising model. The corresponding second-order phase transition will lead to divergences in thermodynamic observables with a power law behavior.

The finite radius of convergence arises from a singularity on the real  $\mu$ -axis only if there exists a  $n_0$  such that for all  $n > n_0$  all expansion coefficients are positive. Since in practice only a few terms in the Taylor series are known such a mathematically rigorous conclusion cannot be drawn in general. The hope is that by investigating the structure of a few known coefficients some hints on the properties of the Taylor series and an estimate for the location of a CEP in the phase diagram can be obtained. Through an inspection of the relative magnitude and relative signs of the expansion coefficients the determination of the radius of convergence of the Taylor series might be possible and the singularity in the complex  $\mu$ -plane which causes the breakdown of this expansion can be located.

Since the thermodynamics in the vicinity of a second-order phase transition is dominated by the singular contribution of the free energy density or thermodynamic potential a generic structure of the Taylor expansion coefficients should occur [25]. At vanishing chemical potential the singular behavior near a phase transition is controlled by the reduced temperature which depends linearly on  $T - T_c$  but quadratically on the chemical potential. Thus, a  $(2n)^{th}$  derivative with respect to  $\mu$  shows a singular behavior that is similar to that of the  $n^{th}$  derivative with respect to temperature. This infers

that the structure of the coefficient  $c_{2n+2}$  can be estimated by investigating the temperature derivative of  $c_{2n}$ . This is indeed found in our model calculations. For an example see Fig. 1 and the discussion in Sec. IV B. This means that  $c_{2n+2}$  will stay positive only up to a temperature which corresponds to the first maximum of the previous coefficient  $c_{2n}$ . Near the transition temperature the coefficients start to oscillate. Thus, through a determination of the first maximum in  $c_{2n}$ , an estimate for the largest temperature below which all coefficients are positive<sup>1</sup>, becomes feasible. Only in this case where all coefficients are positive the corresponding singularity lies on the real axis. Furthermore, this gives an estimate for the critical temperature where a possible CEP in the phase diagram might be located. Once this critical temperature has been obtained the corresponding critical chemical potential follows immediately via  $\mu_c = r(T_c)$ .

At higher temperatures the sign of the Taylor coefficients has no generic structure and the singularity that limits the radius of convergence of the Taylor series will move in the complex  $\mu$ -plane. In this case the convergence radius provides an upper bound since the crossover is related to the real part of the singularity.

For temperatures below the CEP and larger chemical potentials a first-order phase transition emerges. As a consequence, two degenerate minima of the grand potential exist at criticality. Since the Taylor expansion method involves only local information in the vicinity of one minimum of the effective potential, it is, in general, not possible to resolve a first-order phase transition with this technique. However, it still should be possible to give an upper bound for the location of the phase boundary.

### IV. A MODEL ANALYSIS

In this section we apply the Taylor expansion method to an effective  $N_f = 2 + 1$  flavor Polyakov-quark-meson model. This model exhibits a critical endpoint in the  $(T, \mu)$  phase diagram and enables us to inspect the convergence properties of the Taylor series for first-, second-order and crossover phase boundaries. For the first time, the Taylor expansion coefficients are calculated to very high orders, so that the convergence of the series can be probed reliably. Furthermore, the results are confronted with a full model solution.

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<sup>1</sup> As pointed out earlier the mathematically more rigorous criterion for a singularity on the real axis does not rule out the possibility to have a few negative expansion coefficients. We assume here that once a negative coefficient occurs this will lead to irregular signs of the coefficients also in higher orders.



### A. The Polyakov-quark-meson model

The three flavor Polyakov-quark-meson model [26] is a straightforward extension of the two flavor model [27] and serves as an effective model for strongly-interacting matter which incorporates a chiral phase transition, signaled, for example, by a peak in the chiral susceptibility. Through the coupling to the Polyakov loop, which is an order parameter for deconfinement in the infinite quark mass limit, it is also sensitive to deconfining aspects of the QCD phase transition. The thermodynamics of the PQM model is, for vanishing chemical potential evaluated in a mean-field approximation, in good agreement with recent 2 + 1 flavor lattice data [19, 26, 28]. In contrast to lattice simulations, the model can be applied directly at finite chemical potential.

The PQM model Lagrangian reads

$$\mathcal{L}_{\text{PQM}} = \bar{q}(i\mathcal{D} - h\phi_5)q + \mathcal{L}_m - \mathcal{U}(\Phi, \bar{\Phi}), \quad (12)$$

where  $q = (u, d, s)$  denotes the three quark fields. The interaction between the quarks and the mesons is implemented by a flavor-blind Yukawa coupling  $h$ . The meson matrix  $\phi_5 = \sum_{a=0}^8 (\lambda_a/2) (\sigma_a + i\gamma_5 \pi_a)$  consists of nine scalar  $\sigma_a$  and nine pseudo-scalar  $\pi_a$  meson fields.  $\lambda_a$  are the usual Gell-Mann matrices. The covariant derivative  $\mathcal{D} = \mathcal{D} - i\gamma_0 A_0$  couples the Polyakov-loop and its conjugate to the fermionic degrees of freedom where a gauge coupling has been absorbed in the gauge fields. For de-

tails see [27].

The purely mesonic contribution is given by

$$\begin{aligned} \mathcal{L}_m = & \text{Tr} (\partial_\mu \phi^\dagger \partial^\mu \phi) - m^2 \text{Tr} (\phi^\dagger \phi) - \lambda_1 [\text{Tr} (\phi^\dagger \phi)]^2 \\ & - \lambda_2 \text{Tr} (\phi^\dagger \phi)^2 + c (\det(\phi) + \det(\phi^\dagger)) \\ & + \text{Tr} [H(\phi + \phi^\dagger)], \end{aligned} \quad (13)$$

with  $\phi \equiv \sum_a (\lambda_a/2) (\sigma_a + i\pi_a)$ . Chiral symmetry is explicitly broken by the last term in Eq. (13) and the  $U(1)_A$ -symmetry by the 't Hooft determinant term with a constant strength  $c$ . In the 2 + 1 flavor scenario only two order parameters  $\langle \sigma_0 \rangle$  and  $\langle \sigma_8 \rangle$  emerge in the singlet-octet basis. They are conveniently rotated to the non-strange  $\langle \sigma_x \rangle$  and strange  $\langle \sigma_y \rangle$  basis, see [29] for details.

The grand potential evaluated in mean-field approximation is a sum over the mesonic  $U$ , fermionic  $\Omega_{\bar{q}q}$  and Polyakov loop  $\mathcal{U}$  contributions:

$$\Omega = U(\langle \sigma_x \rangle, \langle \sigma_y \rangle) + \Omega_{\bar{q}q}(\langle \sigma_x \rangle, \langle \sigma_y \rangle, \Phi, \bar{\Phi}) + \mathcal{U}(\Phi, \bar{\Phi}), \quad (14)$$

where  $\Phi$  and  $\bar{\Phi}$  denotes the real Polyakov loop expectation values. Note, that at finite chemical potential the  $\Phi$  and  $\bar{\Phi}$  are not linked by complex conjugation and the effective Polyakov loop potential depends on two independent variables.

Explicitly, the quark-anti-quark contribution in presence of the Polyakov loop reads

$$\begin{aligned} \Omega_{\bar{q}q}(\langle \sigma_x \rangle, \langle \sigma_y \rangle, \Phi, \bar{\Phi}) = & -2T \sum_{f=u,d,s} \int \frac{d^3 p}{(2\pi)^3} \left\{ \ln \left[ 1 + 3(\Phi + \bar{\Phi} e^{-(E_{q,f}-\mu)/T}) e^{-(E_{q,f}-\mu)/T} + e^{-3(E_{q,f}-\mu)/T} \right] \right. \\ & \left. + \ln \left[ 1 + 3(\bar{\Phi} + \Phi e^{-(E_{q,f}+\mu)/T}) e^{-(E_{q,f}+\mu)/T} + e^{-3(E_{q,f}+\mu)/T} \right] \right\} \end{aligned} \quad (15)$$

with the flavor-dependent single-particle energies

$$E_{q,f} = \sqrt{k^2 + m_f^2} \quad (16)$$

and quark masses

$$m_l = h \langle \sigma_x \rangle / 2 \quad \text{and} \quad m_s = h \langle \sigma_y \rangle / \sqrt{2} \quad (17)$$

for the light ( $l \equiv u, d$ ) and strange quarks, respectively. In a mean-field approximation, fluctuations are neglected and a divergent vacuum contribution to the grand potential has been omitted here which is irrelevant for our following discussion. See [30] for an investigation of the effect of this vacuum term.

The Yukawa coupling  $h$  is fixed such to reproduce a light constituent quark mass of order  $m_l \approx 300$  MeV. The parameters of the mesonic potential  $U$  are fitted to well-known pseudo-scalar meson masses and decay constants [29]. As in [26] we will employ  $m_\sigma = 600$  MeV.

For the Polyakov-loop part several potentials can be found in the literature which describe the thermodynamics equally well in the vicinity of the chiral transition at  $\mu = 0$ , see e.g. [26]. Here we employ the logarithmic version [31]

$$\begin{aligned} \frac{\mathcal{U}_{\log}}{T^4} = & -\frac{a(T)}{2} \bar{\Phi} \Phi \\ & + b(T) \ln \left[ 1 - 6\bar{\Phi} \Phi + 4(\Phi^3 + \bar{\Phi}^3) - 3(\bar{\Phi} \Phi)^2 \right], \end{aligned} \quad (18)$$

with the temperature-dependent coefficients

$$a(T) = a_0 + a_1 \left( \frac{T_0}{T} \right) + a_2 \left( \frac{T_0}{T} \right)^2, \quad b(T) = b_3 \left( \frac{T_0}{T} \right)^3$$

and the parameter  $T_0 = 270$  MeV. Note that we ignore any  $N_f$ - and/or  $\mu$ -modifications of this parameter here, i.e., the matter back-reaction to the gluon sector, in order to simplify our discussion, see [26, 27, 32] for more details.

Finally, the temperature and  $\mu$ -dependent order parameters are determined by the solution of the gap equations which minimize the grand potential

$$\frac{\partial \Omega}{\partial \sigma_x} = \frac{\partial \Omega}{\partial \sigma_y} = \frac{\partial \Omega}{\partial \Phi} = \frac{\partial \Omega}{\partial \Phi} \Big|_{min} = 0, \quad (19)$$

where  $min$  labels the  $(T, \mu)$ -dependent global minimum of the potential.

### B. Higher-orders Taylor coefficients

Since the grand potential or the pressure are known, the Taylor expansion coefficients in Eq. (2) can be obtained by calculating the corresponding derivatives of the grand potential evaluated at the physical potential minimum. This tedious task is further hindered by the implicit  $\mu$ -dependence of the order parameters, introduced by Eq. (19). The explicit  $\mu$ -dependence is solely given by the fermionic part of the potential  $\Omega_{\bar{q}q}$  whereof the  $\mu$ -derivatives can, in principle, be obtained analytically. However, a fully analytical approach is infeasible since the implicit dependences can only be inverted numerically. Standard numerical derivative techniques such as divided differences may be used for this task at least for the first few derivatives, but definitely fail for higher orders due to the increasing rounding and truncation errors.

In order to proceed a novel derivative technique, based on *algorithmic differentiation* (AD), was developed that properly allows for the implicit dependencies and further avoids numerical errors. The AD technique enables the evaluation of derivatives to high orders even in the case of only numerically solvable implicit dependences, such as in Eq. (19). Furthermore, the derivatives can be obtained with extremely high numerical precision, essentially limited only by machine precision. Details of this method can be found in Ref. [18].

Of course, this AD approach is not limited to simple Taylor series and can also be applied to more involved Taylor expansions of physical quantities which also require temperature-derivatives. An example would be the Taylor expansion of the trace anomaly ( $\epsilon - 3p$ ).

The Taylor coefficients  $c_n$  for the pressure, Eq. (2) have been calculated with this novel AD technique for the three flavor PQM model and can be found, up to the 22<sup>nd</sup> order, in [19]. All coefficients for  $n > 4$  show rapid oscillations near the transition temperature  $T_\chi$  at  $\mu = 0$ . The coefficients become small outside a 5% temperature interval around the  $\mu = 0$  transition temperature  $T_\chi$ , i.e.  $0.95 < T/T_\chi < 1.05$ . Within this temperature interval the amplitudes of the oscillations increase with increasing order and hence higher orders are important even for small expansion parameters, i.e.  $(\mu/T) < 1$ . As an example the coefficient  $c_{12}$  and the properly rescaled temperature derivative of the coefficient  $c_{10}$  are shown in Fig. 1. As already discussed in Sec. III it obeys the same singular behavior as  $c_{12}$ , hence the structure of  $c_{12}$  can

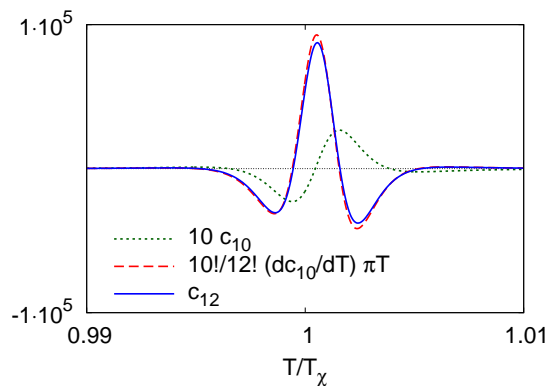


FIG. 1. The Taylor coefficient  $c_{12}$  and the (rescaled) temperature derivative of the coefficient  $c_{10}$  in the vicinity of the critical temperature  $T_\chi$ . For comparison the (rescaled) Taylor coefficient  $c_{10}$  is also shown.

be estimated by the temperature-derivative of  $c_{10}$ . Interestingly, even the magnitude of the coefficient  $c_{12}$  is well estimated by dimensional analysis and compensating the different factorials. Some convergence analysis as well as detailed extrapolations of the pressure and quark number susceptibility Taylor series to finite  $\mu$  with these coefficients can be found in [19].

### C. Determining the phase boundary

We start with a calculation of the  $(T, \mu)$  phase diagram of the PQM model without referring to a Taylor expansion. At vanishing chemical potential the chiral crossover, signaled here by a peak in the chiral susceptibility occurs at  $T_\chi \sim 206$  MeV. At this temperature also the Polyakov loop susceptibility has its maximum. For non-vanishing chemical potentials the position of maxima in both susceptibilities differ. The peak in the Polyakov loop susceptibility occurs at higher temperatures than that in the chiral susceptibility. This scenario changes, however, when fluctuations are taken into account, e.g., if  $\mu$ -corrections of the  $T_0$  parameter in the Polyakov loop potential are considered, see [27, 32]. For small temperatures a first-order chiral phase transition is found which terminates at larger temperature in a CEP. In mean-field approximation the CEP is located at  $(T_c, \mu_c) \sim (185, 167)$  MeV which corresponds to  $T_c \sim 0.9 T_\chi$  and  $\mu_c/T_c \sim 0.9$ . Approximations beyond mean-field push the location of the CEP off the  $T$ -axis. For a mean-field and renormalization group comparison in a quark-meson model, see e.g., [33]. In the following we compare several methods for the determination of the phase boundary with the Taylor coefficients.

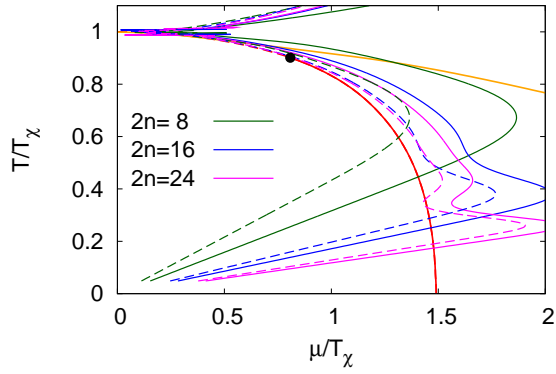


FIG. 2. Estimates for the radius of convergence obtained from  $r_{2n}$  (solid lines) and  $r_{2n-2}^{\chi}$  (dashed lines) for different orders ( $2n = 8, 16, 24$ ) of the Taylor expansion. Also shown are the phase boundaries for the chiral (red line; dashed: crossover, solid: first order) and a deconfinement line identified by the peak position of the Polyakov loop susceptibility (yellow line). The black dot indicates the location of the CEP.

### 1. Taylor expansion

In Fig. 2 we show the results for two estimators for the radius of convergence, obtained from the expansion coefficients of the pressure,  $r_{2n}$  (solid lines), and of the quark number susceptibility,  $r_{2n-2}^{\chi}$  (dashed lines), for three different truncation orders ( $2n = 8, 16, 24$ ) in the  $(T, \mu)$  phase diagram. The phase boundary for the chiral transition and a deconfinement line, corresponding to a maximum in the Polyakov loop susceptibility, are also displayed. Note that the difference in the radii of convergence, estimated from the  $r_{2n}$  and  $r_{2n-2}^{\chi}$ , respectively, is only caused by the prefactor in Eq. (6) since the same Taylor coefficients contribute to both estimators.

Near  $T_{\chi}$  the sign of the expansion coefficients oscillates, indicating that the break down of the series expansion is caused by a singularity in the complex plane away from the real axis. The oscillations in the Taylor coefficients entail oscillations in the radii of convergence at small chemical potentials which are hard to see in Fig. 2. Hence, for small chemical potentials the radius of convergence is not suitable to estimate the phase boundary. For larger values of the chemical potential and for temperatures below  $T_{\chi}$  estimates for the radius of convergence approach the phase boundary from above with increasing truncation order  $n$ . The observed agreement suggests that the singularity limiting the Taylor expansion is close to the real  $\mu$ -axis and the small imaginary part is negligible when compared to the error due to the finite number of coefficients available for a fast crossover. In particular, this is still valid for the region in the vicinity of the CEP. We note that for  $n \gtrsim 10$  corrections to the asymptotic value  $r$  are well described in terms of  $\mathcal{O}(1/n)$  corrections. In fact, with an ansatz  $r(1 + A/n)$  for the estimators of the radius of convergence  $r_{2n}$ , the leading  $\mathcal{O}(1/n)$  cor-

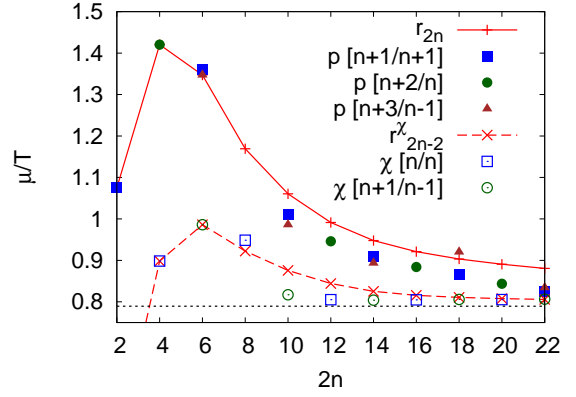


FIG. 3. Estimate of the phase boundary at  $T = 190 \text{ MeV} \sim 0.92 T_{\chi}$  with  $r_{2n}$  and  $r_{2n}^{\chi}$  and poles in the Padé approximation of the pressure and quark number susceptibility as a function of the order of the Taylor expansion  $2n$ . The used highest coefficient is  $c_{2n+2}$ . The dotted horizontal line indicates the phase boundary calculated directly at finite  $\mu$ . Note also that an estimate is possible only for even Padé approximations.

rections can be eliminated by using subsequent estimates. This leads to estimates for  $r$  obtained from the pressure and quark number susceptibility series that agree within a few percent and reach the asymptotic value within 15% for  $2n > 14$ . The coefficient  $A$  for the correction term, obtained in this way, is about a factor 5 larger in the pressure series than in the quark number susceptibility series. Qualitatively, this different asymptotic behavior of both series can be understood in terms of the structure of the singular contribution to the grand potential that limits the radius of convergence. We discuss this in more detail in the Appendix A.

At low temperatures the estimates for the radius of convergence increase with increasing order  $n$  of the Taylor expansion and allow also ratios  $\mu/T > 1$ . This is in agreement with the small magnitude of the higher order coefficients in this temperature region. In this region the results are in agreement with results from the resonance gas (cf. [16]), i.e. the estimates of the convergence radius of the pressure are given by  $r_{2n}^{\text{HRG}}(T) = 1/3\sqrt{(1+2n)(2+2n)}$ .

As already mentioned above, it is not possible to resolve a first-order transition with the Taylor expansion. Therefore,  $r_{2n}$  as well as  $r_{2n}^{\chi}$  yield estimates for the radius of convergence that are larger than the true location of the first-order transition line and signal a misleading convergence of the Taylor expansion. In this region the Taylor expansion might provide stable and continuous results but one cannot extract the precise position of the boundary for a first-order phase transition.

## 2. Padé approximation

The Padé approximation could improve the convergence behavior and therefore provide a better estimate of the phase boundary since the Padé approximant employs all Taylor coefficients in contrast to the previous analysis where only two subsequent Taylor coefficients enter. The pole in the  $[N/2]$  Padé approximation yields the corresponding radius of convergence as described in Sec. II C. For a general  $[N/M]$  Padé approximation we use the first pole at real and positive  $\mu$  in order to estimate the phase boundary. Since all Taylor coefficients with their corresponding error enter in the Padé approximant the error propagation is more involved here in contrast to the previous discussion where only two error sources enter. In this context, the application of the Padé approximation in lattice simulations is much more involved. However, in the model analysis the coefficients, obtained with the AD technique, exhibit extremely small numerical errors and result in a stable and reliable Padé approximation.

Apart from the diagonal scheme  $[N/N]$  we also use a non-diagonal  $[N + 2/N]$  approximation for the susceptibility and a  $[N + 2/N - 2]$ , respectively  $[N + 2/N]$  approximation for the pressure and determine always the first pole at real and positive  $\mu$ .

In Fig. 3 we show for a fixed temperature  $T = 0.92 T_\chi$  the estimates of the phase boundary extracted from Padé approximations for the pressure ( $p$ ) and the quark number susceptibility ( $\chi$ ) for different truncation orders  $n$ . The chosen temperature is slightly above the temperature of the CEP in the phase diagram. In addition, the estimates for the radii of convergence ( $r_{2n}$  and  $r_{2n}^\chi$ ) and the chiral crossover chemical potential (dashed horizontal line) are also shown. For small truncation orders  $2n \leq 8$  the  $[N/2]$  Padé approximations coincide with the radii of convergence as expected. For  $2n > 8$  we observe that the Padé approximation converges faster for the pressure as well as for the susceptibility compared to the radii of convergence obtained without the Padé approximation.

We conclude that the Padé approximation converges faster at larger truncation orders, in particular for the quark number susceptibility. The estimate of the phase boundary from the Padé approximation becomes comparable to the one obtained from estimators for the radius of convergence determined directly from ratios of Taylor expansion coefficients only at significantly larger truncation order. For example, in Fig. 3 the distance of the Padé estimate to the horizontal line at  $2n = 12$  is achieved with the Taylor expansion only for  $2n \geq 20$ . However, the lower truncation order in the Padé approximation induces a more involved error propagation. This is no problem with the AD-techniques but might hamper lattice simulations.

*a. First-order transition* As already mentioned, the Taylor expansion around  $\mu = 0$  fails if a first-order phase transition emerges since the jump to a new global minimum of the effective potential cannot be resolved. However, it might still be possible to enter the metastable

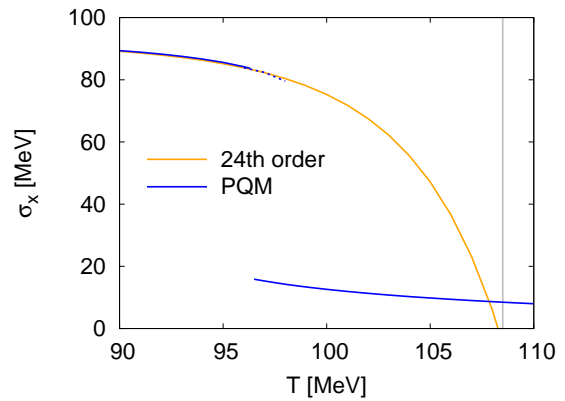


FIG. 4. Taylor expansion of the (non-strange) order parameter  $\sigma_x$  compared to the direct evaluation at finite  $\mu$  for  $\mu/T = 3$ . The dotted lines indicate the beginning of the metastable phase. The vertical line indicates the estimate for the radius of convergence,  $r_{24}$ .

phase with the Taylor expansion method. In this case the radius of convergence just reflects the fact that this expansion is still valid in the metastable phase. However, a precise determination of the first-order transition is not possible. This conceptual drawback is not modified when the Padé approximation is employed.

As an example we show in Fig. 4 for  $\mu/T = 3$  the chiral order parameter, the non-strange condensate  $\sigma_x$ , as a function of the temperature in the vicinity of a first-order transition. Here  $\sigma_x$  has been obtained from a Taylor series truncated at 24<sup>th</sup> order. The lines, labeled with PQM, represent the full model solution of the gap equation Eq. (19) where a first-order transition can be resolved. Both solutions agree very well in the low temperature phase until  $T \sim 96$  MeV. The dotted line indicates the begin of the metastable phase. One sees that it is still possible to enter this metastable phase with the Taylor expansion method. The vertical line in the figure marks the location of the estimate for the radius of convergence obtained for the chosen  $n = 24$  truncation order. Furthermore, this example also demonstrates that the Taylor expansion method is applicable also for  $\mu/T > 1$  as long as one stays within the convergence regime.

*b. Critical endpoint* Directly at the critical endpoint a second-order phase transition emerge and no discontinuity in the order parameter appears. Hence, the radius of convergence might be well-suited to estimate the location of the critical endpoint in the phase diagram once the critical temperature is known. The corresponding critical chemical potential can again be obtained via

$$\mu_c = r(T_c) = \lim_{n \rightarrow \infty} r_n(T_c). \quad (20)$$

From the discussion given so far and from Fig. 3 one may conclude that at fixed temperature the radius of convergence can be estimated with an accuracy of about 15%-20% from a series of the order  $\mathcal{O}(\mu^{12})$ . This is clearly an acceptable uncertainty in view of the difficulties one



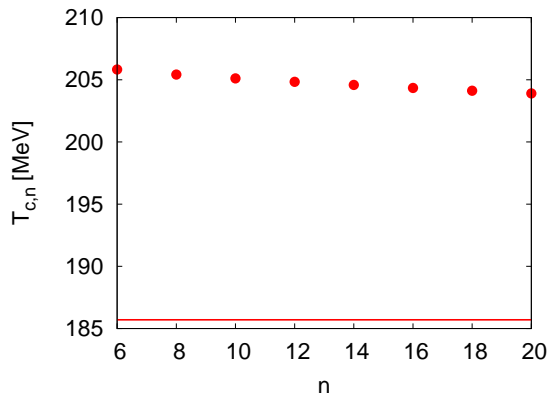


FIG. 5. Temperature  $T_{c,n}$  at which the Taylor coefficients  $c_n$  becomes negative for different truncation orders  $n$ . The solid horizontal line denotes the critical temperature of the CEP.

has to face in current QCD calculations with non-zero chemical potential.

However, the determination of  $T_c$  is still a non-trivial task. A criterion is needed, that allows to estimate at a given order of the expansion the temperature regime in which all expansion coefficients may stay positive as discussed in Sec. III. As an example we show the zeros of the Taylor series of the pressure in the complex  $\mu/T$ -plane around a temperature point where a coefficient changes its sign in Appendix B.

In Fig. 5 we plot the temperature  $T_{c,n}$  defined as the temperature where the Taylor coefficient  $c_n$  becomes negative for different truncation orders. This yields an upper bound for the critical temperature. Of course, in the limit  $n \rightarrow \infty$  the temperature series of these approximations should approach the critical temperature of the CEP, i.e.,

$$T_c = \lim_{n \rightarrow \infty} T_{c,n}. \quad (21)$$

However, at least with our model analysis, only a very slow convergence of the estimators for the critical temperature at the CEP is visible. Even at high truncation order of 20<sup>th</sup> there is still a temperature difference of the order of 20 MeV which is why we do not reconsider Eq. (20).

In addition, this convergence behavior might be improved by applying the Padé approximation but the identification of a proper convergence criterion is more involved as discussed in Appendix B.

## V. SUMMARY AND CONCLUSIONS

The convergence properties of the Taylor expansion method which is used to extend lattice QCD calculations to non-zero chemical potential have been investigated. The method has been applied to an effective  $N_f = 2 + 1$  flavor Polyakov-quark-meson model and the results obtained with the Taylor expansion have been compared to

a full model mean-field solution. By means of a novel algorithmic differentiation technique higher-order Taylor coefficients could be calculated for the first time. As a function of the temperature the coefficients start to oscillate in the vicinity of the phase transition region. The number of roots and magnitude of the oscillations increase with the coefficient order. Two definitions of the radius of convergence, one through the pressure series coefficients and the other one via the corresponding susceptibility coefficients have been discussed. The convergence of the estimators for the radius of convergence of the susceptibility series is faster than the corresponding one for the pressure series.

With the Padé approximation the convergence rate could be further improved. By investigating the pole structure of the Padé approximant a definition for the radius of convergence could be extracted and a better estimate for the phase boundary could be achieved.

While the convergence radius yields the precise location of the phase boundary only for a second-order transition, i.e., at the critical endpoint, we observed a good agreement of the convergence radius with the full model solution also for temperatures above  $T_c$ . In view of the error of convergence radius due to the finite number of coefficients the convergence radius can provide a valuable estimate also for the location of a rapid crossover where the limiting singularity is close to the real axis in the complex  $\mu$ -plane.

The singularity lies on the real axis only in the case where all coefficients are positive. This criterion also provides an estimate for the critical temperature  $T_{c,n}$ . In our study this estimate depends only weakly on the truncation order. But even for truncation orders above 20<sup>th</sup> there is still a significant gap to the full model solution and a precise determination of the location of the CEP remains open. Note that the error in estimating  $T_c$  also affects the estimation of  $\mu_c$ .

Although, the situation may be different in model calculations and in QCD, our study suggests that for a meaningful application of the Taylor method to lattice QCD higher order Taylor coefficients are definitely necessary in order to control systematically truncation errors in the series expansion and to estimate reliably the location of a possible critical endpoint in the QCD phase diagram. At present the available number of coefficients extracted in lattice QCD calculations is not sufficient to locate a critical endpoint in the QCD phase diagram with the Taylor expansion method. However, if the critical endpoint is located at smaller temperatures a broader temperature interval is expected to emerge in which the Taylor coefficients will oscillate. The estimators for the critical temperatures  $T_{c,n}$  are then expected to show a stronger temperature dependence and they should decrease faster. However, in this case also the CEP may be located at large values of  $\mu/T$  and higher orders in the expansion may be needed due to this.

Furthermore, when going beyond mean-field approximations in our model calculation, quantum and thermal

fluctuations in the hadronic phase will surely modify the oscillations of the Taylor coefficients. This too may improve the estimate of the critical temperature with the Taylor expansion method. However, also in this case the location of a possible CEP is shifted towards the  $\mu$ -axis [34] and more coefficients are necessary for an adequate description. To explore this quantitatively we plan to extend the present study beyond mean-field as well as tightening the AD techniques with functional renormalization group methods.

With the Taylor expansion method it is in general not possible to describe a first-order transition completely including the precise determination of the critical temperature since only information about one potential minimum are available. One may, however, establish upper bounds for the location of the phase boundary.

### ACKNOWLEDGMENT

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### Appendix A: Asymptotic behavior of Taylor expansion coefficients

The QCD critical point is expected to belong to the universality class of the three dimensional Ising model. The critical behavior in the vicinity of this point is controlled by two couplings which characterize fluctuations in thermal and magnetic (symmetry breaking) directions of the effective Ising Hamiltonian. The chemical potential will mix with both couplings [35]. When approaching the critical point in the  $(T, \mu)$ -plane the dominant singular contributions to, e.g., the quark number susceptibility arise from the magnetic coupling. When approaching the critical endpoint in the QCD phase diagram at fixed temperature, the quark number susceptibility thus is expected to scale like [33, 35, 36]

$$\chi_q(T, \mu)/T^2 \sim (1 - \mu/\mu_c)^{1/\delta-1} = (1 - \mu/\mu_c)^{\gamma/\beta\delta} \quad (\text{A1})$$

which arises from a singular term in the grand potential, i.e., the pressure which has the form,

$$(p/T^4)_{\text{sing}} \sim (1 - \mu/\mu_c)^{1+1/\delta}. \quad (\text{A2})$$

Assuming that these singular terms give indeed the dominant contribution to the Taylor expansion coefficients at

high order, we obtain for the asymptotic behavior of the estimators for the radius of convergence ( $r \equiv \mu_c$ ) of the pressure and quark number susceptibility series, respectively,

$$\begin{aligned} r_{2n} &\sim \mu_c \left( 1 + \frac{2\delta + 1}{2n\delta} \right) \\ r_{2n}^{\chi} &\sim \mu_c \left( 1 + \frac{1}{2n\delta} \right). \end{aligned} \quad (\text{A3})$$

We thus expect that in comparison to the pressure series, corrections to the radius of convergence are smaller in the quark number susceptibility series. In mean-field approximation, which is used in our current study, the relative factor is  $2\delta + 1 = 7$  and it is about 10.6 in the three dimensional Ising model. Indeed, this seems to be realized with the series discussed in this study, although the approach to the asymptotic value is slow.

### Appendix B: Roots in the complex $\mu/T$ -plane

As mentioned in Sec. III a singularity in the complex  $\mu/T$ -plane limits the radius of convergence of a Taylor expansion. In Fig. 6 an example of the root distribution in the complex  $\mu/T$ -plane of a 16<sup>th</sup> order Taylor series of the pressure is given. The temperatures in the three panels are chosen such that the highest Taylor coefficient  $c_{16}$  changes sign while all the remaining coefficients stay positive. In the left panel  $c_{16}$  is still positive. As expected all 16 roots are complex and distributed on a circle whose radius corresponds to the radius of convergence  $r_{16}$ . For  $c_{16} = 0$  (middle panel) the Taylor polynomial is of degree 14 and consequently only 14 roots emerge. Approaching  $c_{16} = 0$  from positive values the two root pairs which are each closest to the imaginary axis merge to each one purely imaginary root and the other root vanishes at imaginary plus or minus infinity. When the temperature is further increased, i.e.,  $c_{16}$  becomes negative (right panel), two roots reenter the complex  $\mu/T$ -plane on the real  $\mu$ -axis from plus or minus infinity and rapidly approach the radius of convergence.

A similar analysis could also be performed with the Padé approximation which shows, in general, a more rapid convergence behavior. However, the investigation for this case is more involved since two polynomials occur and possible root cancellations can emerge which are hard to distinguish numerically from real roots. In addition, deeper problems may further arise since the CEP is related to a pole with a non-integer critical exponent which is generally difficult to describe properly within a Padé approximation.

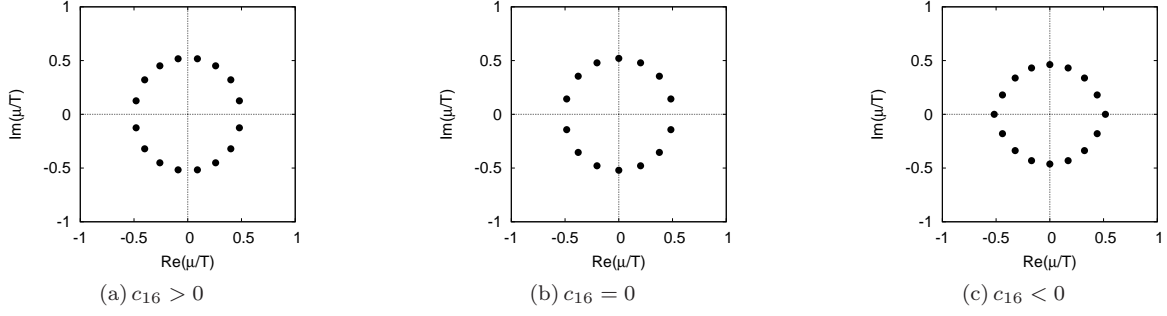


FIG. 6. Root distribution in the complex  $\mu/T$ -plane of a 16<sup>th</sup> order Taylor series of the pressure. The corresponding temperatures in the three panels are chosen such that the highest Taylor coefficient  $c_{16}$  changes sign while all the remaining Taylor coefficients are still positive.

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